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A STUDY OF THE PEAK OZONE LEVELS IN THE TORONTO AREA

RAC Project No. 474C

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1. BACKGROUND

The concentration of ozone in the Toronto area exceeds Ontario's regulatory limit more often than any other pollutant. During the year Ontario's Air Quality Index was first introduced, (June 1988 to May 1989), Shenfeld and Yap (1989) reported that between 80 and 95% of the hours that the Air Quality Index was in the Moderate to Poor range within Metropolitan Toronto, ozone was the major pollutant. Furthermore, during the summer of 1988, the ozone hourly averages were frequently well above 120 ppb, (AQI=50), which is known to cause an impact on health to a large percentage of the population, especially those who may be exercizing outdoors. These high ozone developments occurred during periods of long-range transport (LRT) of ozone and precursors into the Province from the United States. During the summer of 1989, the occurrences of high ozone readings were much less frequent, as the LRT contributions were not as prevalent, even during ozone conducive weather such as warm, sunny and light wind/calm conditions.

Kurtz et al. (1989) have utilized the long-range transport Acid Deposition and Oxidant Model (A.D.O.M) to show the influence of U.S. emissions of nitrogen oxides and reactive hydrocarbons to the levels of ozone in Southern Ontario. Air mass back trajectory studies, most recently by Yap et al. (1988) established that U.S. sources of these pollutants were

responsible for much of the high ozone values reported in Southern Ontario.

Ozone studies by Shenfeld (1977), Mukammel et al. (1982), and more recently Yap et al. (1988), established the meteorological conditions required for the development of high ozone levels in Southern Ontario. Studies of ozone developments in other geographical locations by Revlett (1978), Wolff and Lioy (1978), Prior et al. (1981), Simpson et al. (1983), and Robeson and Steyn (1990) have established that peak hourly average levels of ozone can be correlated to specific meteorological parameters.

2. STUDY OBJECTIVES

The main objective of this study is to determine the proportion of the peak ozone levels in Toronto resulting from the LRT of ozone and precursors into Toronto. A second objective is to determine whether the relationship between peak ozone levels and meteorological parameters can be used to predict the peak ozone levels and hence the Air Quality Index for the afternoon and early evening. The third objective is to determine the relationship between the peak hour ozone level and the maximum 8-hour running average of ozone the same day and what levels of 8-hour averages relate to peak hour levels of 80 ppb (Moderate air quality) and 120 ppb (Poor air quality).

3. STUDY DESCRIPTION

For this study, we have selected the peak hour ozone levels during each day from May to September inclusive, for the years 1988 and 1989, during which the Pearson International Airport reported temperatures equal to or exceeding 23°C and the cloud cover was equal or less than four tenths opacity. The selected days were then separated into days that LRT occurred from the industrial States and those that it did not. This classification was determined by using synoptic weather maps and the Ontario Ministry of the Environment Air Resources Branch archives of the 48-hour back trajectories of air into Toronto.

Three Metropolitan Toronto ozone recording locations were selected for study, namely; Downtown Toronto (Breadalbane), Scarborough (Lawrence and Kennedy) and North York (Yonge and Finch).

For LRT and non-LRT days, multiple regression equations are used to relate the peak ozone levels at each of the above locations with the Pearson International Airport maximum temperature, average wind speed and average cloud cover during the hours of 9AM to 4PM. Another dependent variable used, is the peak hour ozone level measured the previous day at the rural station outside Simcoe, Ontario. The difference between the peak ozone levels determined from equations with LRT and with non-LRT

is used to determine the contribution of ozone to the Metropolitan Toronto locations due to LRT.

4. REGRESSION ANALYSIS

A multiple regression analysis was completed for the three sites (Toronto, Scarborough and North York) for each of LRT and non-LRT days. A simple regression equation was derived from the ozone data set of the Ontario Ministry of the Environment:

$$Y = B_0 + B_1 *X_1 + B_2 *X_2 + B_3 *X_3 + B_4 *X_4 \qquad (1)$$

where:
- Y - Maximum Ozone Level (PPM)
- X_1 - Maximum Temperature (°C)
- X_2 - Average Wind Speed (Km/hr)
- X_3 - Average Cloud Opacity (10^{th}'s)
- X_4 - Previous Day's Maximum Ozone (PPM) Recorded at Simcoe, Ontario

The results of the regression analysis are outlined in Table 1.

The partial regression coefficients derived from equation (1) are not independent of the particular metrics used for the variables and are therefore not directly comparable. Each one gives the rate of change of the dependent variable for a unit change of the particular independent variable while the remaining independent variables are held statistically constant. It is, however, possible to standardize the partial regression

TABLE 1 : MULTIPLE REGRESSION EQUATIONS
MAXIMUM OZONE LEVEL PREDICTION
(MAY 1988 to SEPTEMBER 1989)

The Regression Equation is of the form:

$$Y = B_0 + B_1 * X_1 + B_2 * X_2 + B_3 * X_3 + B_4 * X_4$$

Y - Maximum Ozone Level (PPM)
X_1 - Maximum Temperature (C)
X_2 - Average Wind Speed (Km/hr)
X_3 - Average Cloud Opacity (10^{th}s)
X_4 - Previous Day's Maximum Ozone (PPM) Recorded at Simcoe (22071)

	TORONTO (31104) [LRT]	TORONTO (31104)	SCARBOROUGH (33033) [LRT]	SCARBOROUGH (33033)	NORTH YORK (34020) [LRT]	NORTH YORK (34020)
N	35	41	36	42	30	35
B_0	-71.798	-54.829	-59.189	-23.973	-66.524	-27.924
B_1	5.166	3.931	4.985	3.333	5.335	3.381
B_2	-1.026	-0.894	-1.330	-1.088	-1.047	-0.949
B_3	-0.524	-1.625	-0.679	-2.525	-1.902	-1.413
B_4	0.152	0.115	0.125	0.099	0.109	0.051
R	0.805	0.679	0.698	0.653	0.685	0.696
R^2	0.648	0.461	0.487	0.427	0.470	0.485
SE	15.410	19.777	17.515	19.556	21.621	12.941
Y	72.818	55.133	76.111	56.000	77.268	57.241
X_1	29.230	26.380	29.229	26.350	29.461	26.938
X_2	14.153	13.128	13.952	12.886	14.231	15.257
X_3	1.923	1.895	1.880	1.862	2.177	1.801
X_4	72.659	55.967	72.756	56.563	74.146	57.931

N - Number of Observations
B_0 - Multiple Regression Coefficient (intercept)
B_1 - Multiple Regression Coefficient (for X_1)
B_2 - Multiple Regression Coefficient (for X_2)
B_3 - Multiple Regression Coefficient (for X_3)
B_4 - Multiple Regression Coefficient (for X_4)
R - Correlation Coefficient
R^2 - R-Squared
SE - Standard Error of the Estimate (PPB)
Y - Mean Measured Ozone (PPB)
X_1 - Mean Maximum Temperature (C)
X_2 - Mean Average Wind Speed (Km/hr)
X_3 - Mean Average Cloud Opacity
X_4 - Mean Previous Day's Measured Ozone at Simcoe (PPB)

coefficients with new values represented as b_j's, derived as follows (King, 1969):

$$b_j = B_j \frac{\sigma_j}{\sigma_o} \qquad (2)$$

where σ_j and σ_o are the standard deviations of the independent and dependent variables respectively. Since they are dimensionless items, the b_j's can be compared directly as measures of the relative importance of the different variables in accounting for the variation in the dependent variable. The b_j's for each site is found in Table 2.

In all cases, the most important variable is air temperature. For the LRT cases, air temperature is about 3 times more important in the regression equation than the next most important variable, wind speed. The importance of wind speed in the regression for non-LRT cases, however, is not much less than that of air temperature. Cloud opacity and the previous day's ozone play the smallest role in the regression equation, however, their inclusion provides some improvement in the prediction.

The overall significance of the multiple regression can be tested by an analysis of variance. This test is equivalent to testing the null hypothesis that in the population from which the observations have been sampled, there is no significant regression of the dependent on the independent variables. The test consists of determining the F ratio for each case, that is

TABLE 2 : STANDARDIZED REGRESSION COEFFICIENTS AND ANALYSIS OF VARIANCE TEST (MAY 1988 to SEPTEMBER 1989)

	TORONTO (31104) [LRT]	TORONTO (31104)	SCARBOROUGH (33033) [LRT]	SCARBOROUGH (33033)	NORTH YORK (34020) [LRT]	NORTH YORK (34020)
b_1	0.699	0.587	0.603	0.567	0.650	0.505
b_2	-0.197	-0.347	-0.242	-0.488	-0.189	-0.370
b_3	-0.037	-0.156	-0.045	-0.282	-0.120	-0.133
b_4	0.144	0.139	0.111	0.040	0.098	0.062
σ_1	3.633	3.136	3.592	3.069	3.661	3.151
σ_2	5.389	8.163	5.410	8.093	5.422	8.211
σ_3	1.981	2.013	1.997	2.019	1.903	2.020
σ_4	26.516	25.428	26.687	24.764	27.011	25.622
σ_r	28.048	20.983	29.687	18.032	30.015	21.103
F	14.375*	6.279*	8.653*	6.088*	10.161*	6.622*

b_1 = Standardized Regression coefficient (X_1)
b_2 = Standardized Regression coefficient (X_2)
b_3 = Standardized Regression coefficient (X_3)
b_4 = Standardized Regression coefficient (X_4)
σ_1 = Standard Deviation for X_1
σ_2 = Standard Deviation for X_2
σ_3 = Standard Deviation for X_3
σ_4 = Standard Deviation for X_4
σ_r = Standard Deviation for Y

F = F - Ratio

* Significant at 5 % level of confidence

the ratio of the mean square of the sum of squares of the regression over the mean square of the sum of squares of the residual. If the computed F exceeds the tabled value for a selected level of confidence, then the null hypothesis is rejected.

The F ratio is found at the bottom of Table 2. In all cases, the null hypothesis can be rejected at 5% level of confidence.

The effect of LRT from the industrial United States can be determined, at any particular site, from the difference in the predicted ozone levels using identical values for the independent variables in both the LRT and non-LRT regression equations. This difference was determined by using the above equations and all combinations of: air temperature being equal to 23, 27, 30 and 34 degrees C, wind equal to 0, 5, 10 and 20 km/hr., cloud cover equal to 0, 2, and 4 tenths, and the previous day's ozone equal to 40, 60, 80, 100 and 120 ppb. The results showed a minimum increase due to LRT to be 24.2% (13.7 ppb), a maximum increase of 48.7% (38.1 ppb) and an average of 31.7% (25.9 ppb). However, it can be expected that the effect of LRT to increase ozone concentrations would be even greater than indicated in this analysis which does not take into account the difference in the previous day's ozone levels during LRT and non-LRT days. The mean of the previous day's ozone is 15 ppb larger during LRT than

non-LRT days (see Table 1) and all of the regression equations are positively correlated with the previous day's ozone.

5. MODEL TEST

The multiple regression equation, as a predictor of peak level ozone, was tested by using independent data sets from May to September 1987 for the Toronto and Scarborough sites. Measured peak ozone levels were compared against predicted peak ozone levels by using the appropriate regression equation, the relevant meteorology and the measured previous day's ozone at Simcoe. Figures 1 to 4 show graphs of measured versus predicted zone levels for each of LRT and non-LRT cases at Toronto and Scarborough while Figure 5 shows the total measured versus predicted graph.

Willmott (1982), citing several examples showing that real significance and statistical significance do not exhibit a close correspondence, has proposed measures of 'systematic' and 'unsystematic' error to examine the types of differences and an 'index of agreement' to investigate the relative size of differences. Because a model should explain most of the major trends present in the observed record, it is important to know what proportion of RMSE is systematic ($RMSE_s$) and what proportion is unsystematic ($RMSE_u$). In this fashion, with respect to a 'good' model, $(RMSE_s)^2$ should approach zero while $(RMSE_u)^2$ should approach RMSE. The 'index of agreement' (D) was proposed to

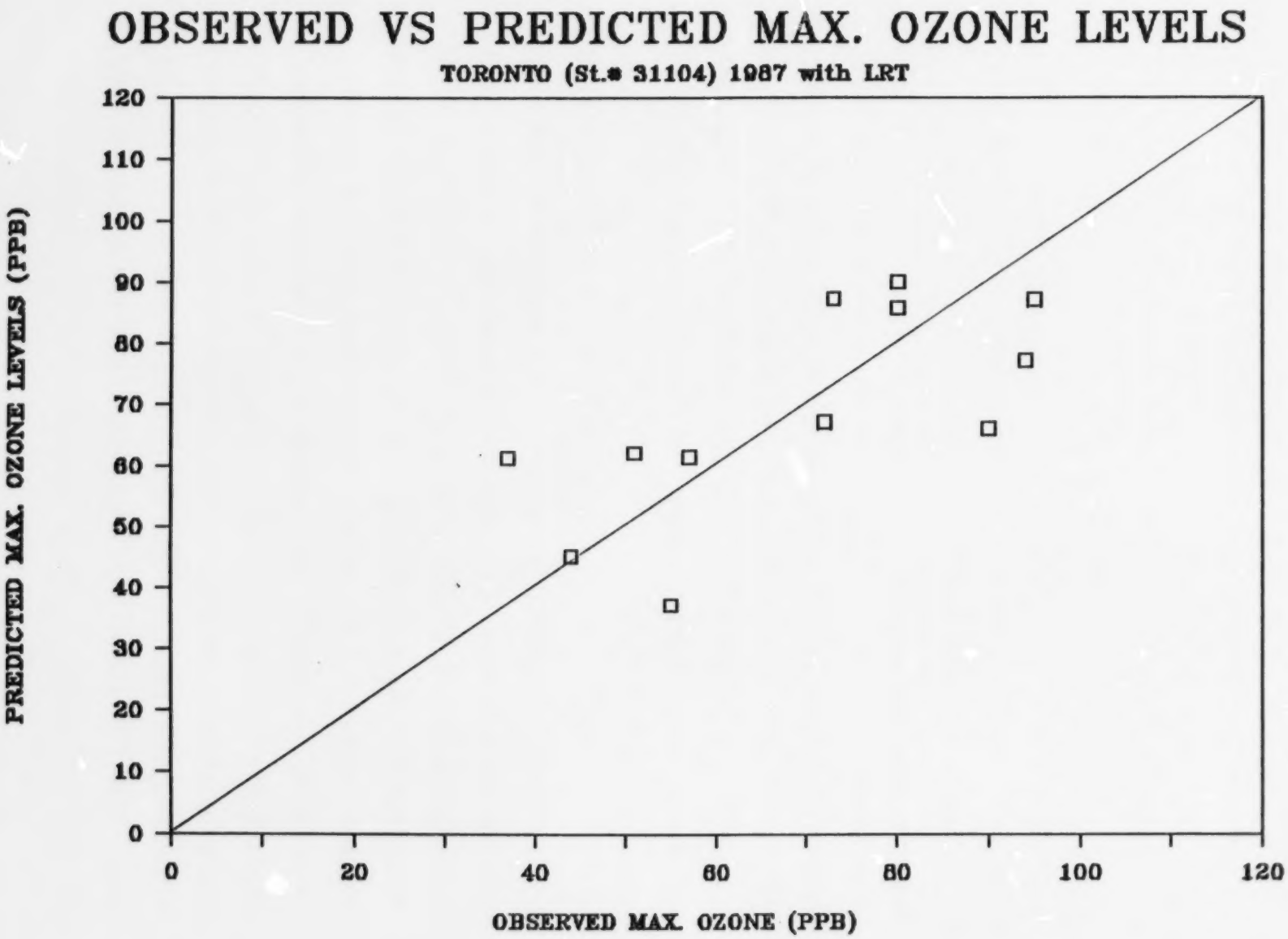

FIGURE 1: Observed Versus Predicted Maximium Ozone Levels, Toronto 1987 with LRT

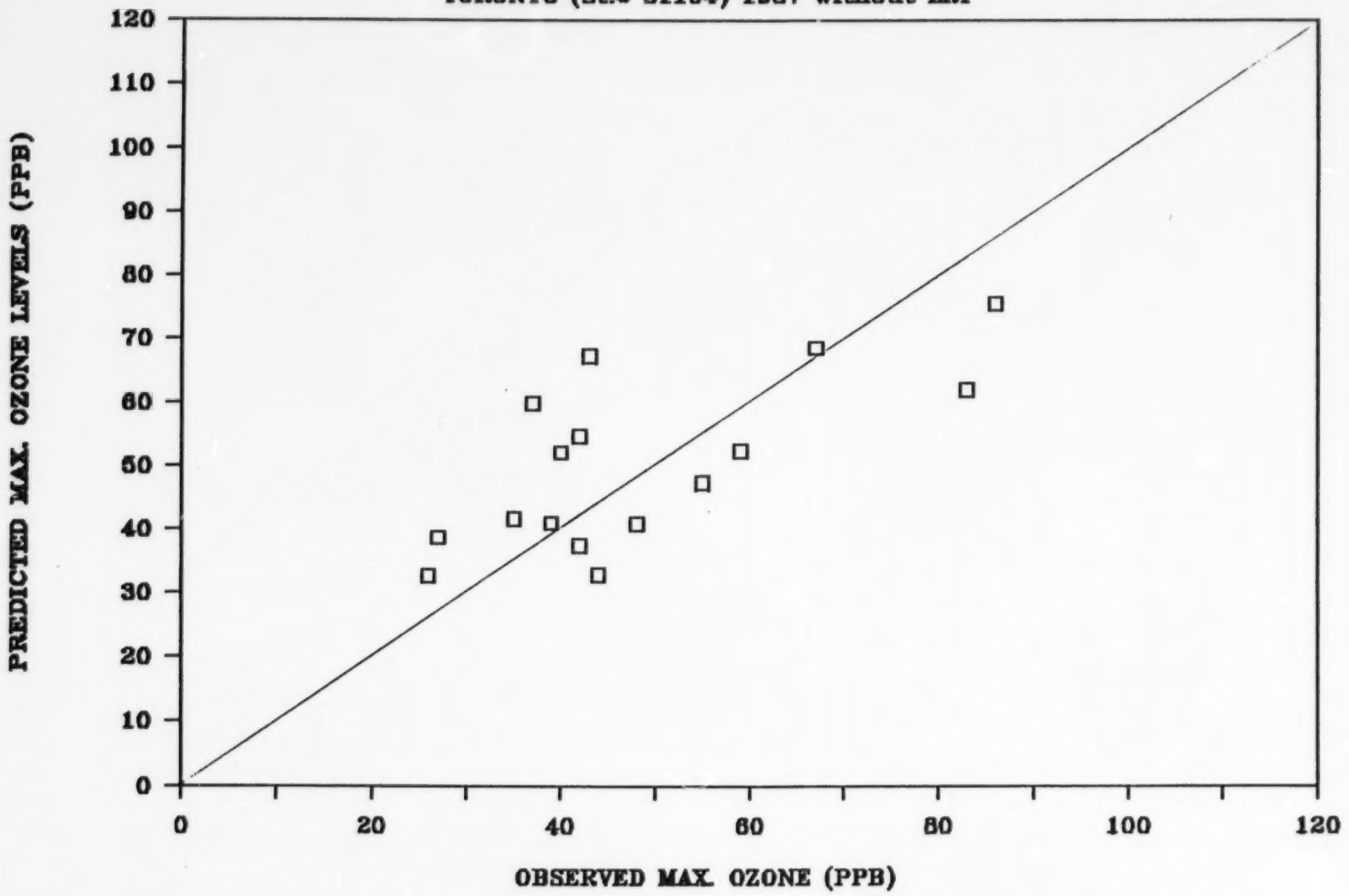

FIGURE 2: Observed Versus Predicted Maximium Ozone Levels, Toronto 1987 without LRT

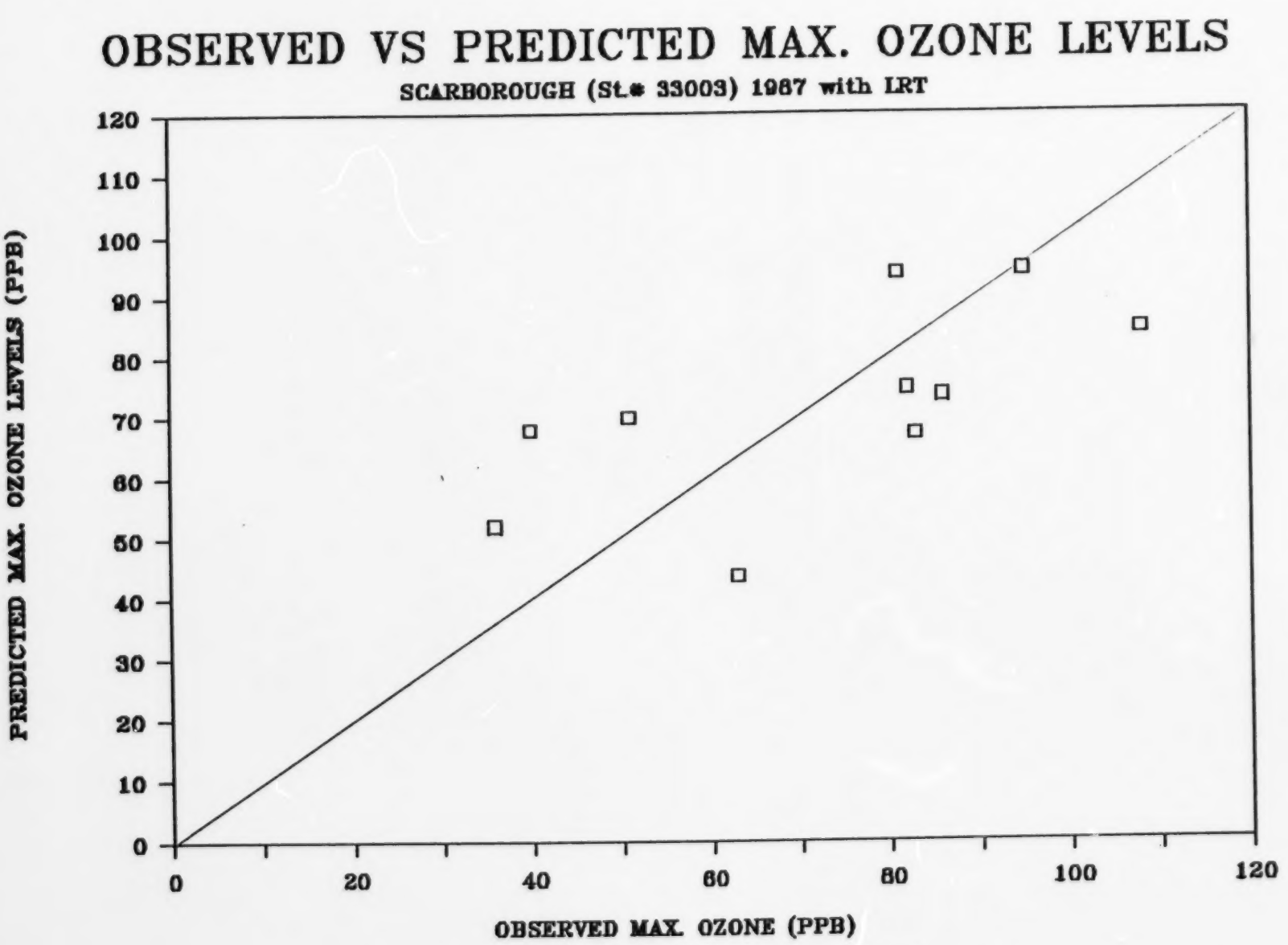

FIGURE 3: Observed Versus Predicted Maximium Ozone Levels, Scarborough 1987 with LRT

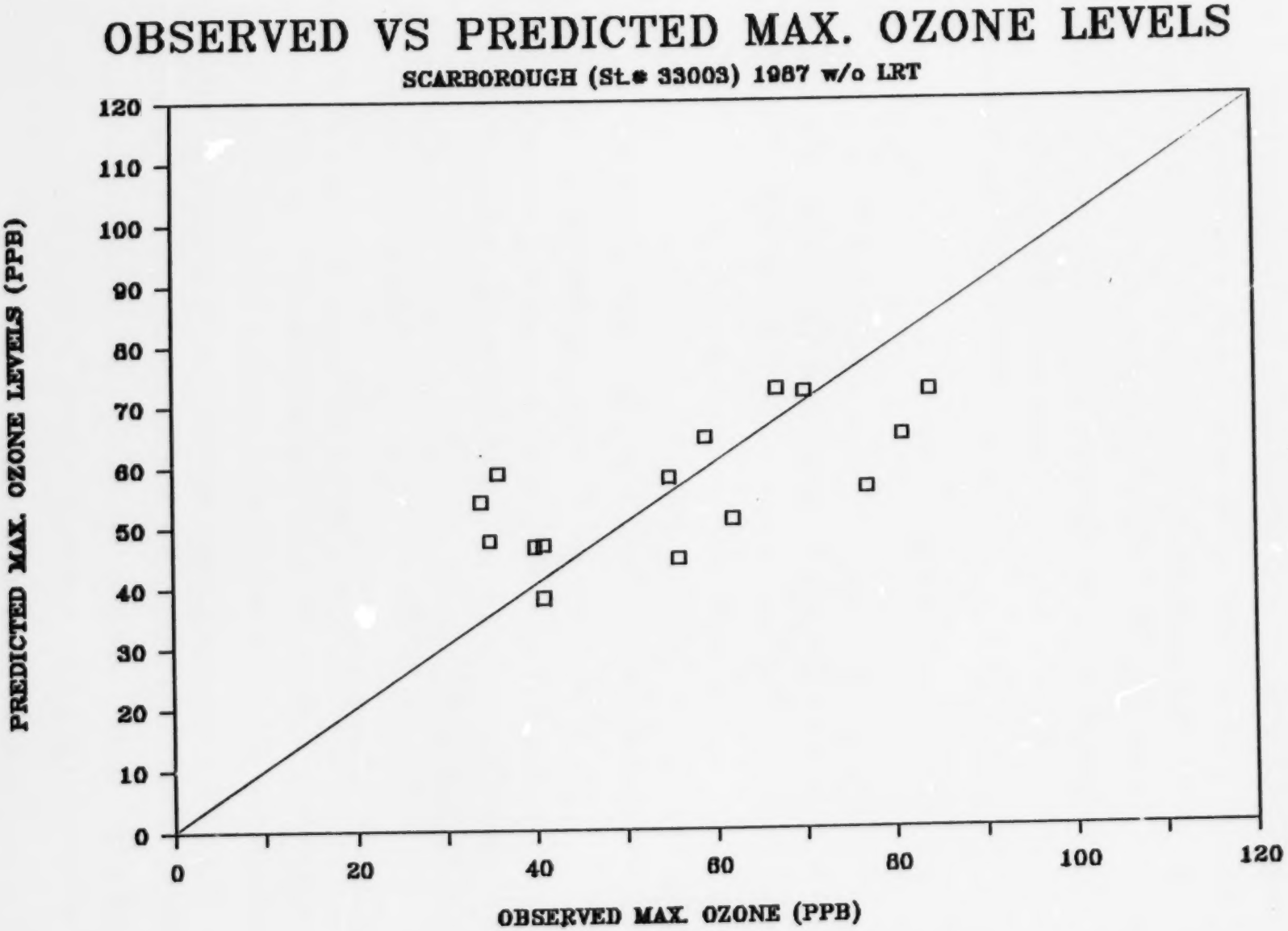

FIGURE 4: Observed Versus Predicted Maximium Ozone Levels, Scarborough 1987 without LRT

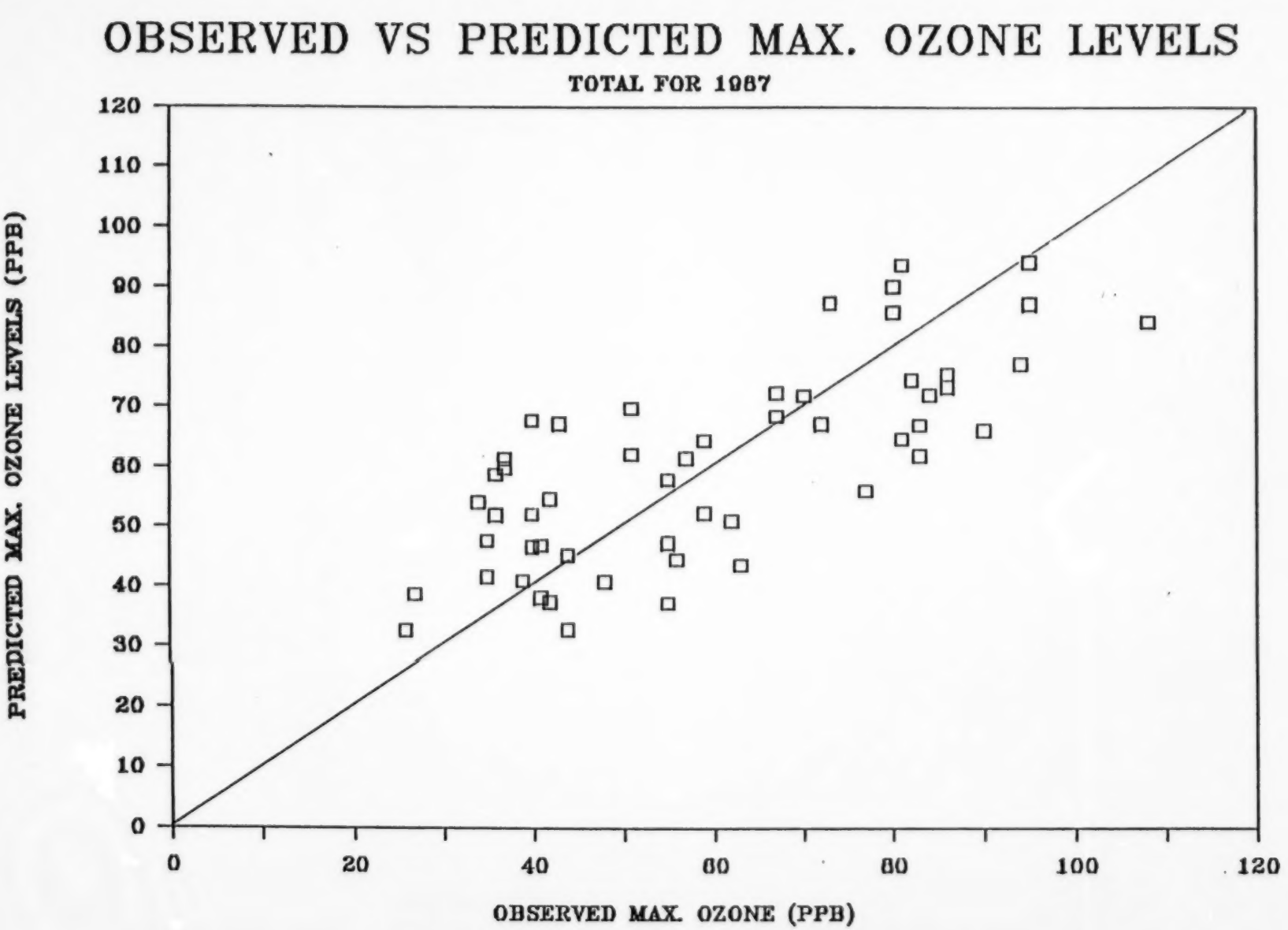

FIGURE 5: Observed Versus Predicted Maximium Ozone Levels, Total 1987

yield a measure of the relative size of differences; this index is intended to be a descriptive measure which is both relative and bounded ($0 \leq D \leq 1$) and can be widely applied in order to make cross-comparisons between models. As the agreement between the observed and predicted variables increases, D approaches 1.0 . Table 3 shows the equations used to calculate model performance.

Table 4 contains the model performance statistics. It should first be noted that the calculated and measured population means and standard deviations are very similar, in fact in no case is the difference between the two means greater than 2 ppb.

The MAE and RMSE indicate a mean difference between the predicated and observed values of approximately 13 ppb. With the unsystematic portion of the RMSE being around 10 ppb, this indicates that most of the RMSE is unsystematic and it need not be assumed that there is a missing independent variable in the regression analysis.

The last column of Table 4 contains the model performance statistics for the combined "computed versus. measured" matrix. This is included to increase the size of the population to be 'large' (N>30) since the general utility of such indices as RMSE is questionable as N becomes small (Willmott, 1982). The high value of the Willmott Index of Agreement (D) (0.853) indicates a

TABLE 3: Statistical Measures of Model Performance (after Willmot, 1982)

I. SUMMARY STATISTICS:

1. Mean Observed: $$\bar{O} = N^{-1} \sum_{i=1}^{N} O_i$$

2. Mean Predicted: $$\bar{P} = N^{-1} \sum_{i=1}^{N} P_i$$

3. Standard Deviation (Observed): $$S_o = \left[N^{-1} \sum_{i=1}^{N} (O_i - \bar{O})^2 \right]^{1/2}$$

4. Standard Deviation (Predicted): $$S_p = \left[N^{-1} \sum_{i=1}^{N} (P_i - \bar{P})^2 \right]^{1/2}$$

5. Intercept (a) and Slope (b) of the Least Squares Regression: $$\hat{P}_i = a + b\, O_i$$

II. DIFFERENCE STATISTICS:

6. Mean Biased Error: $$MBE = N^{-1} \sum_{i=1}^{N} (P_i - O_i)$$

7. Mean Absolute Error: $$MAE = N^{-1} \sum_{i=1}^{N} |P_i - O_i|$$

8. Root Mean Square Error: $$RMSE = \left[N^{-1} \sum_{i=1}^{N} (P_i - O_i)^2 \right]^{1/2}$$

9. Root Mean Square Systematic Error: $$RMSE_S = \left[N^{-1} \sum_{i=1}^{N} (\hat{P}_i - O_i)^2 \right]^{1/2}$$

10. Root Mean Square Unsystematic Error: $$RMSE_U = \left[N^{-1} \sum_{i=1}^{N} (P_i - \hat{P}_i)^2 \right]^{1/2}$$

11. Index of Agreement:

$$D = 1 - \left[\sum_{i=1}^{N} (P_i - O_i)^2 \Big/ \sum_{i=1}^{N} (|P_i - \bar{O}| + |O_i - \bar{O}|)^2 \right], \quad 0 \le D \le 1$$

TABLE 4 : OZONE LEVEL PREDICTION
MODEL PERFORMANCE STATISTICS

	TORONTO [LRT]	TORONTO	SCARBOROUGH [LRT]	SCARBOROUGH	TOTAL
N	12	16	11	15	54
O	69.000	48.312	73.273	55.866	60.092
P	69.112	50.291	74.004	56.517	61.033
S_o	19.821	17.647	22.865	17.410	21.198
S_p	17.102	13.424	16.714	10.907	16.915
a	0.603	0.528	0.470	0.422	0.604
b	27.512	24.757	39.547	32.953	24.755
MBE	0.112	1.978	0.731	0.650	0.940
MAE	11.872	10.557	15.256	10.556	11.806
RMSE	13.928	12.498	16.816	12.479	13.794
$RMSE_s$	7.537	8.295	11.572	9.747	8.376
$RMSE_u$	11.713	9.348	12.201	7.791	10.959
R^2	0.488	0.483	0.413	0.453	0.573
D	0.821	0.816	0.764	0.763	0.853

N - Number of Observations
O - Average Observed Ozone
P - Average Predicted Ozone
S_o - Observed Standard Deviation
S_p - Predicted Standard Deviation
a - Slope of Regression Line (OBS vs PRED)
b - Intercept of Regression Line
MBE - Mean Bias Error
MAE - Mean Absolute Error
RMSE - Root Mean Square Error
$RMSE_s$ - Systematic Portion of RMSE
$RMSE_u$ - Unsystematic Portion of RMSE
R^2 - R-Squared
D - Wilmott Index of Agreement

reasonably good agreement between the predicted and measured peak ozone levels.

6. 8-HOUR AVERAGE OZONE LEVELS

The final part of this study deals with the relationship between the peak hourly ozone level and the 8-hour average on the same day. The data set used for the determination of the regression equations is used here to determine the linear regression between the 8-hour average (Y) and the peak hourly average (X_o) by the equation:

$$Y = B_o + B_1 * X_1 \qquad (2)$$

Table 5 shows the linear regression equation for each site and for each of LRT and non-LRT days. From the table we can see a high level of correlation with an average correlation coefficient (R) of 0.95 and an average coefficient of determination (R^2) of 0.89 . Using these linear equations it is possible to estimate the 8-hour average associated with a peak hourly ozone level of 80 ppb (Moderate air quality) and 120 ppb (Poor air quality). These values are listed in Table 5 and are equal to, on average, 62 and 91 ppb, respectively. Figures 6 to 11 show graphs of the 8-hour average ozone level versus the maximum ozone level for each of LRT and non-LRT cases at Toronto, Scarborough and North York while Figure 12 shows the total 8-hour average versus maximum ozone graph.

TABLE 5 : LINEAR REGRESSION EQUATIONS
8 HOUR AVERAGE OZONE LEVEL PREDICTION
(MAY 1988 to SEPTEMBER 1989)

The Regression Equation is of the form:

$$Y = B_o + B_1 * X_1$$

Y - 8 Hour Average Ozone (PPM)
X_1 - Peak Hourly Ozone (PPM)

	TORONTO (31104) [LRT]	TORONTO (31104)	SCARBOROUGH (33033) [LRT]	SCARBOROUGH (33033)	NORTH YORK (34020) [LRT]	NORTH YORK (34020)
N	35	41	36	42	30	35
B_o	0.495	10.177	1.886	4.479	-4.196	5.210
B_1	0.772	0.631	0.766	0.682	0.855	0.714
R	0.985	0.943	0.943	0.964	0.945	0.948
R^2	0.918	0.889	0.889	0.930	0.893	0.899
SE	5.993	5.430	6.296	5.220	8.512	5.244
Y	56.152	41.379	59.494	41.941	62.383	45.610
X_1	72.818	55.133	76.111	56.000	77.268	57.241
MOD. LEVEL	62.225	60.657	63.166	59.039	64.204	62.330
POOR LEVEL	93.135	85.897	93.806	86.319	98.404	90.810

N - Number of Observations
B_o - Linear Regression Coefficient (intercept)
B_1 - linear Regression Coefficient (for X_1)
R - Correlation Coefficient
R^2 - R-Squared
SE - Standard Error of the Estimate (PPB)
Y - Mean 8 Hour Average Ozone (PPB)
X_1 - Mean Peak Hourly Ozone (C)
MOD. LEVEL - Value of 8 Hour Average Calculated for a Peak Ozone Level of 80 PPB
POOR LEVEL - Value of 8 Hour Average Calculated for a Peak Ozone Level of 120 PPB

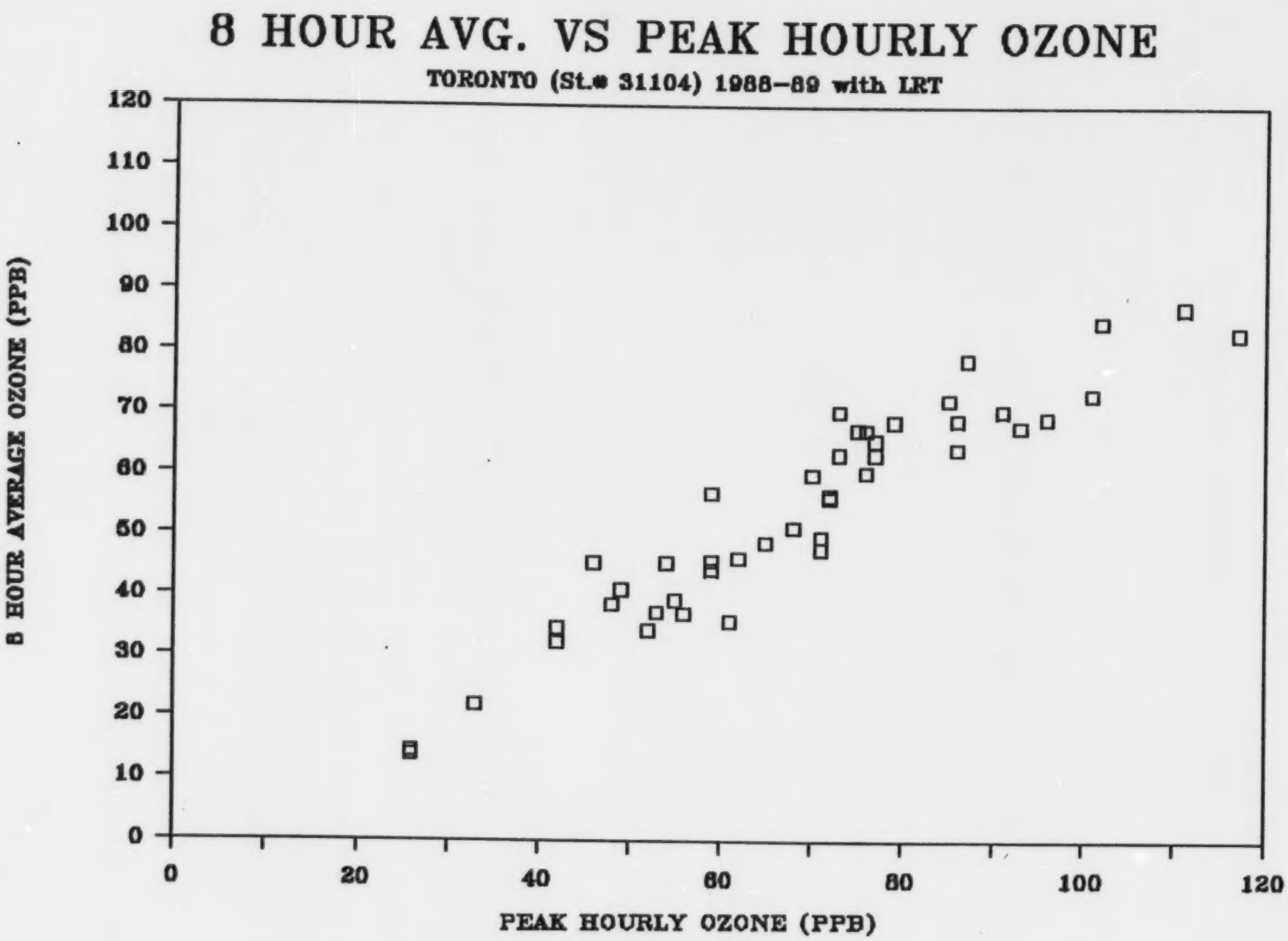

FIGURE 6: 8 Hour Average Versus Peak Hourly Ozone
Toronto, 1988-89 with LRT

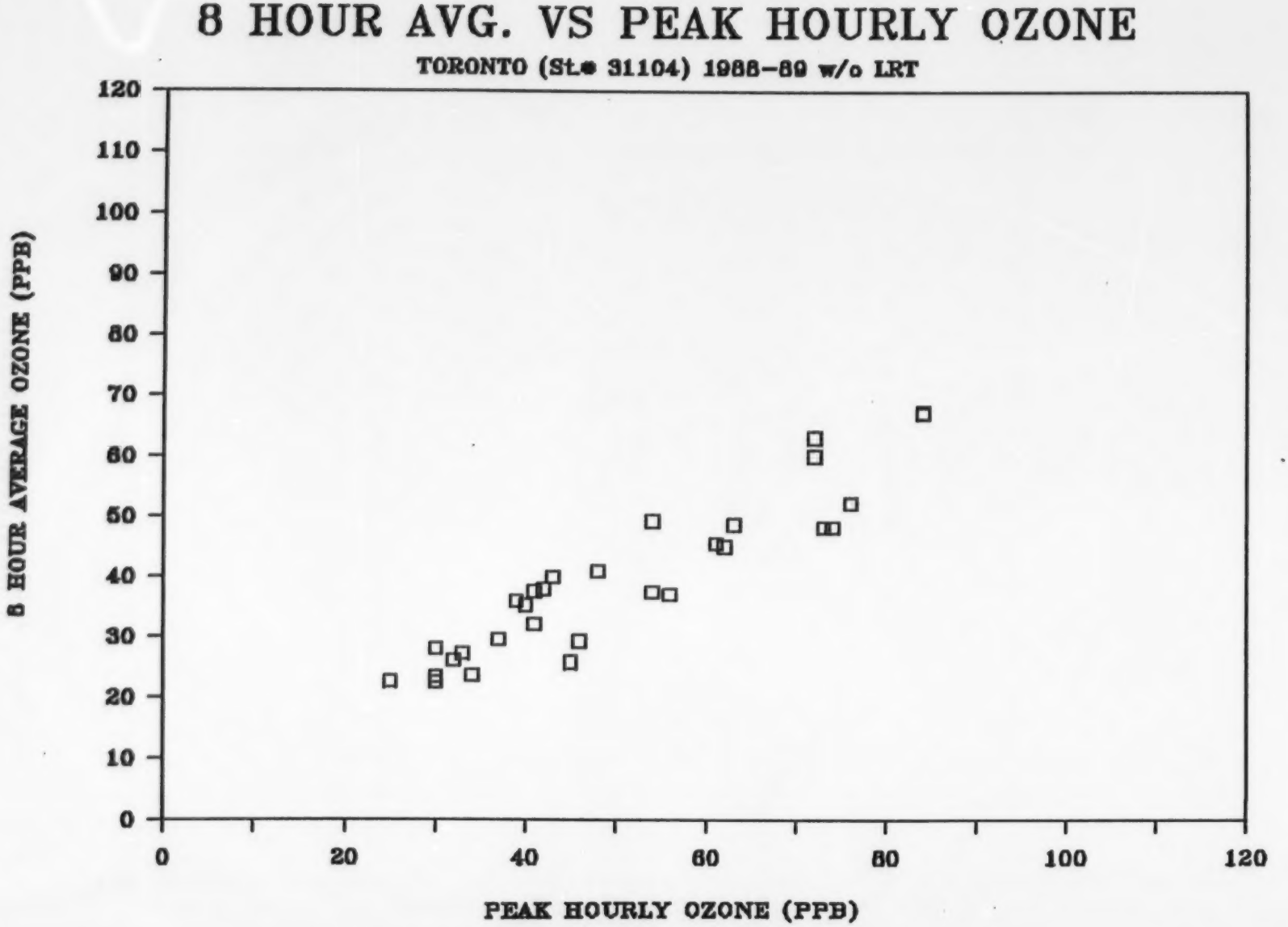

FIGURE 7: 8 Hour Average Versus Peak Hourly Ozone
Toronto, 1988-89 without LRT

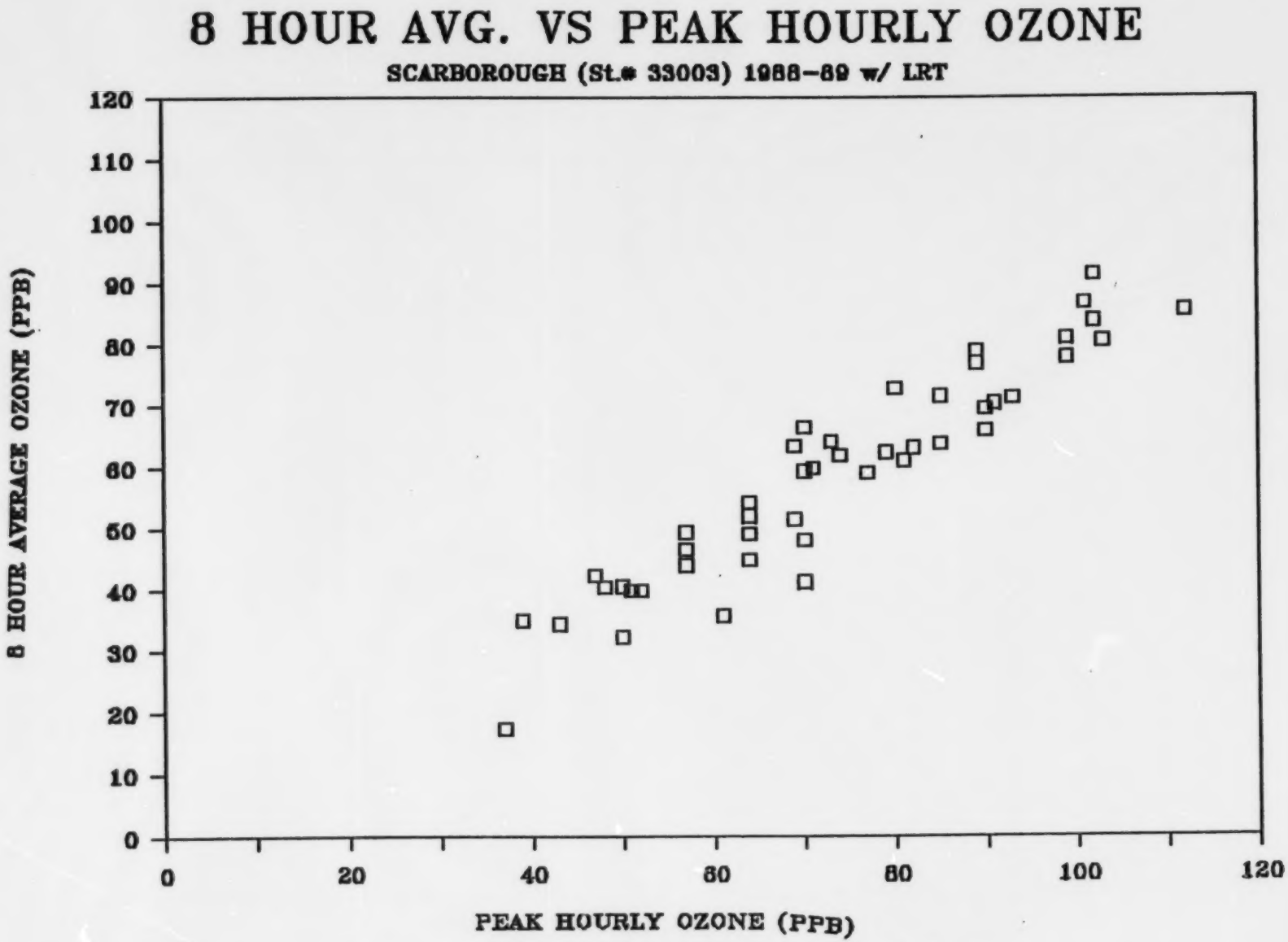

FIGURE 8: 8 Hour Average Versus Peak Hourly Ozone
Scarborough, 1988-89 with LRT

8 HOUR AVG. VS PEAK HOURLY OZONE

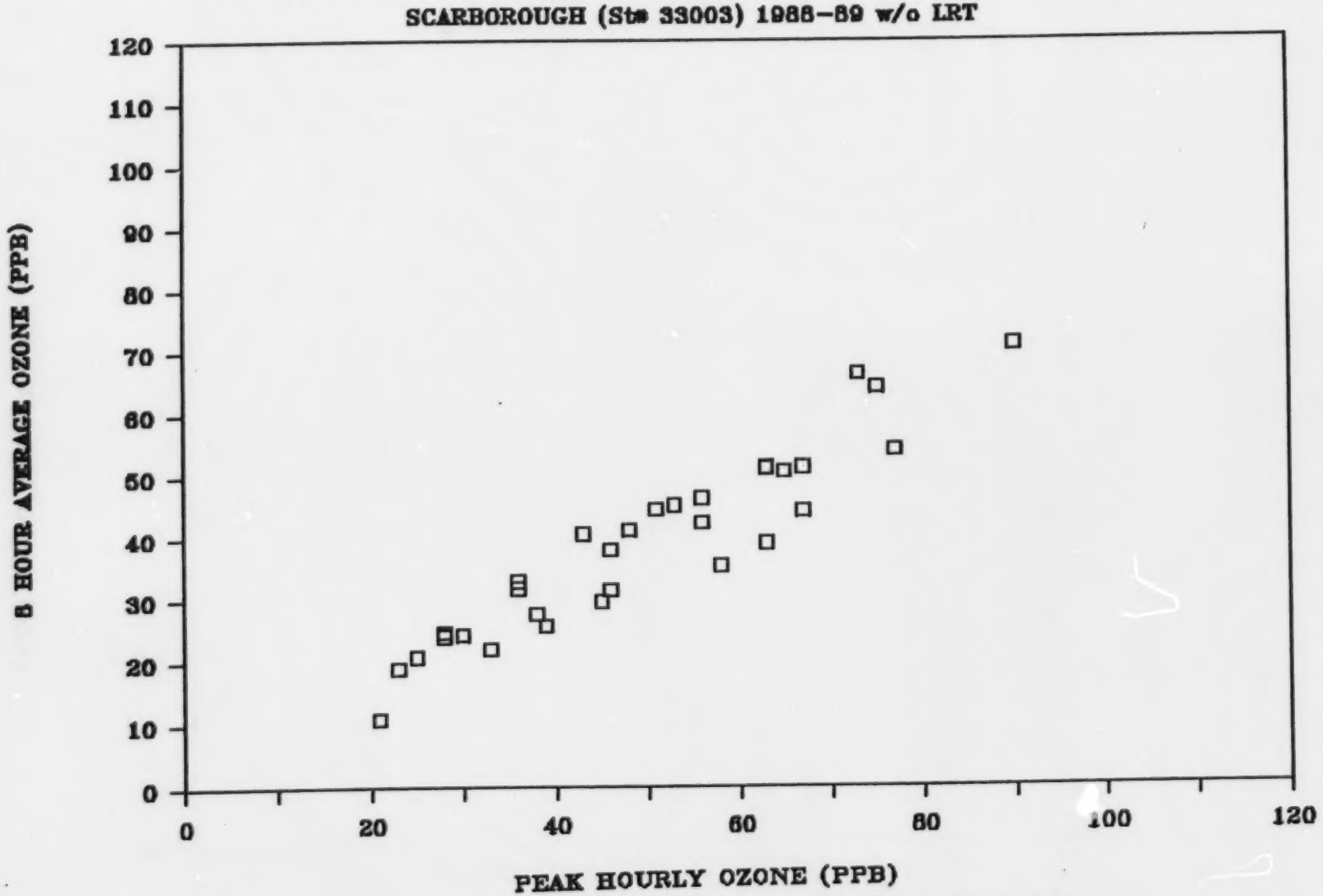

FIGURE 9: 8 Hour Average Versus Peak Hourly Ozone
Scarborough, 1988-89 without LRT

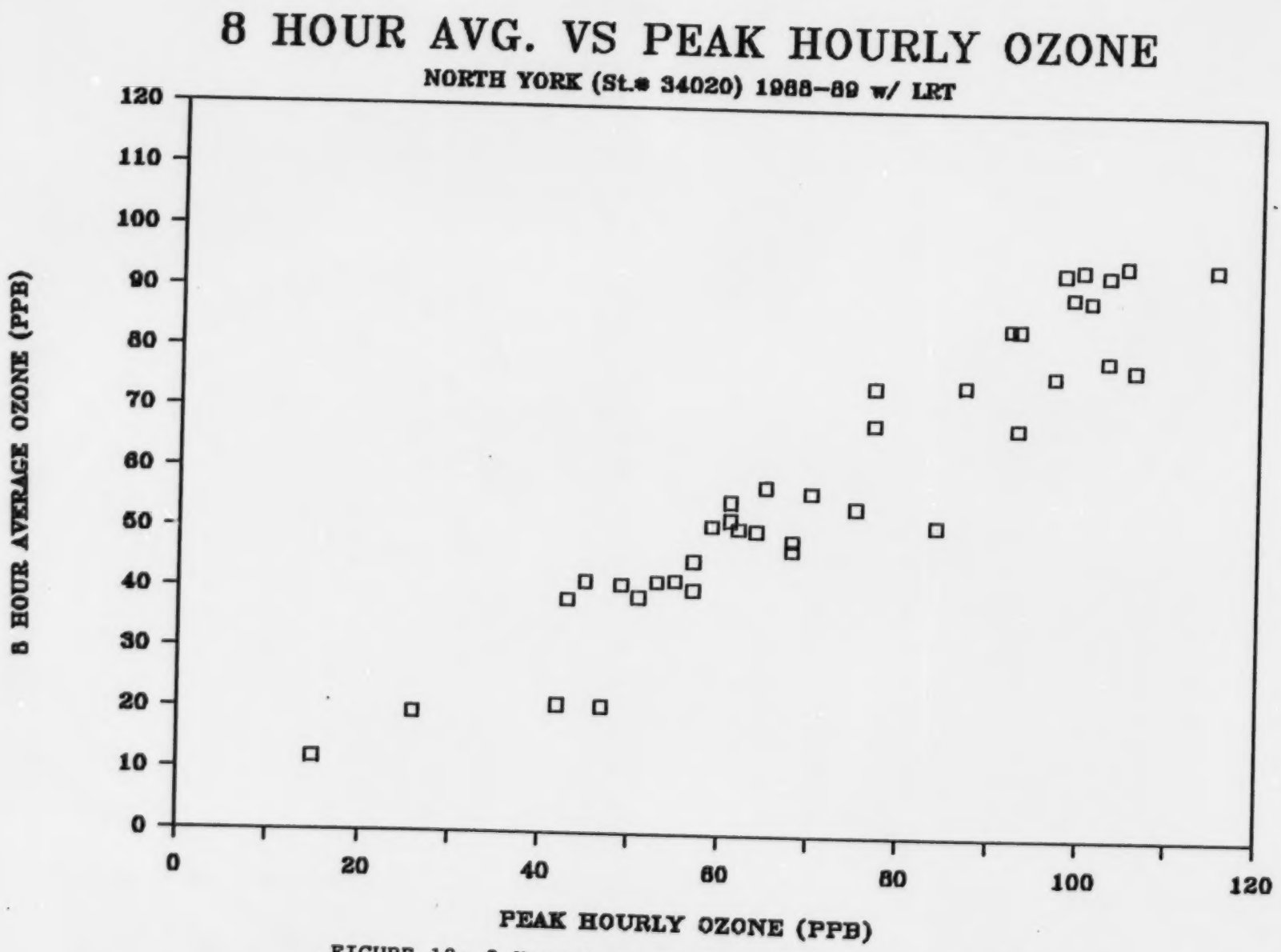

FIGURE 10: 8 Hour Average Versus Peak Hourly Ozone
North York, 1988-89 with LRT

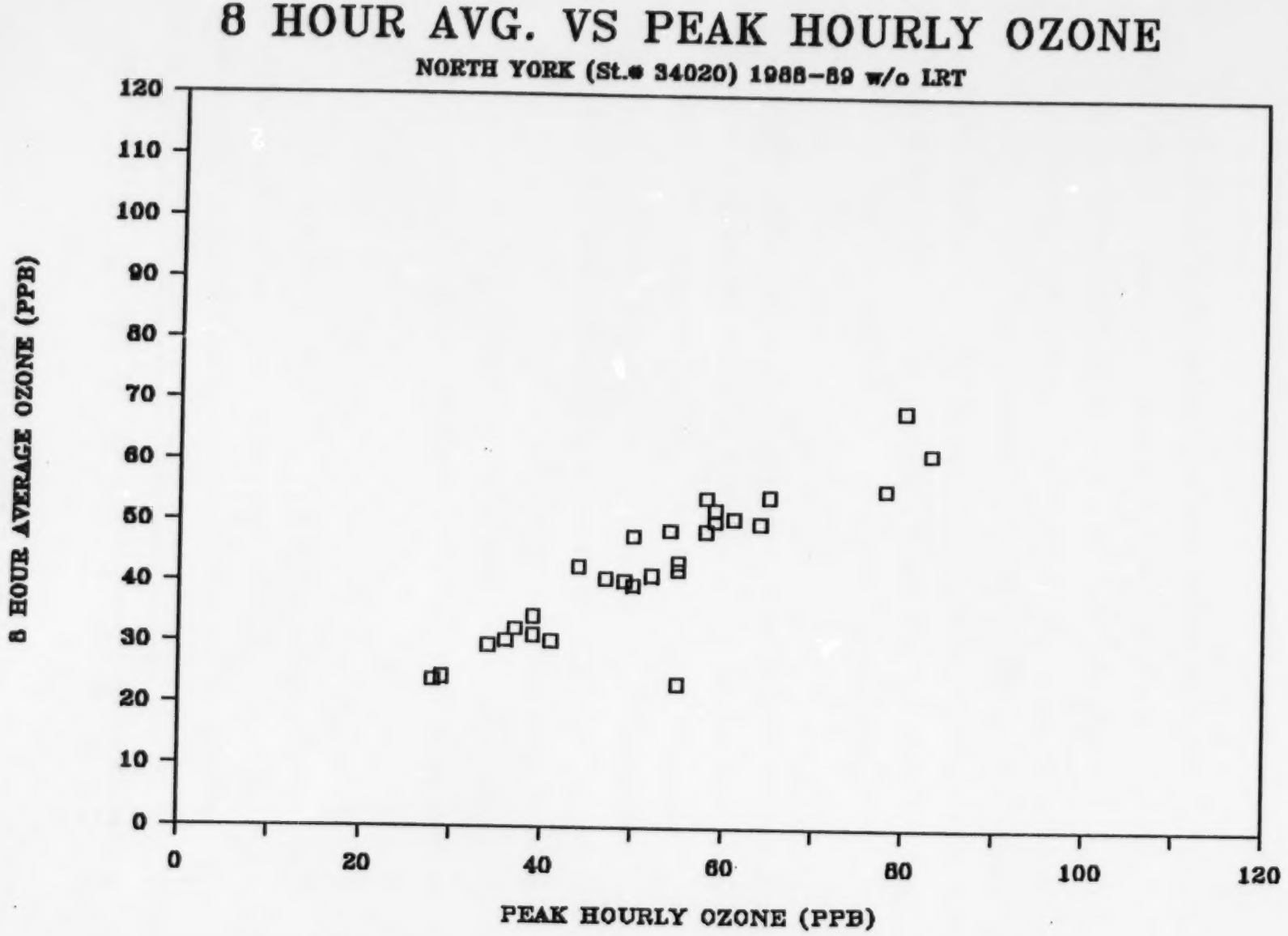

FIGURE 11: 8 Hour Average Versus Peak Hourly Ozone
North York, 1988-89 without LRT

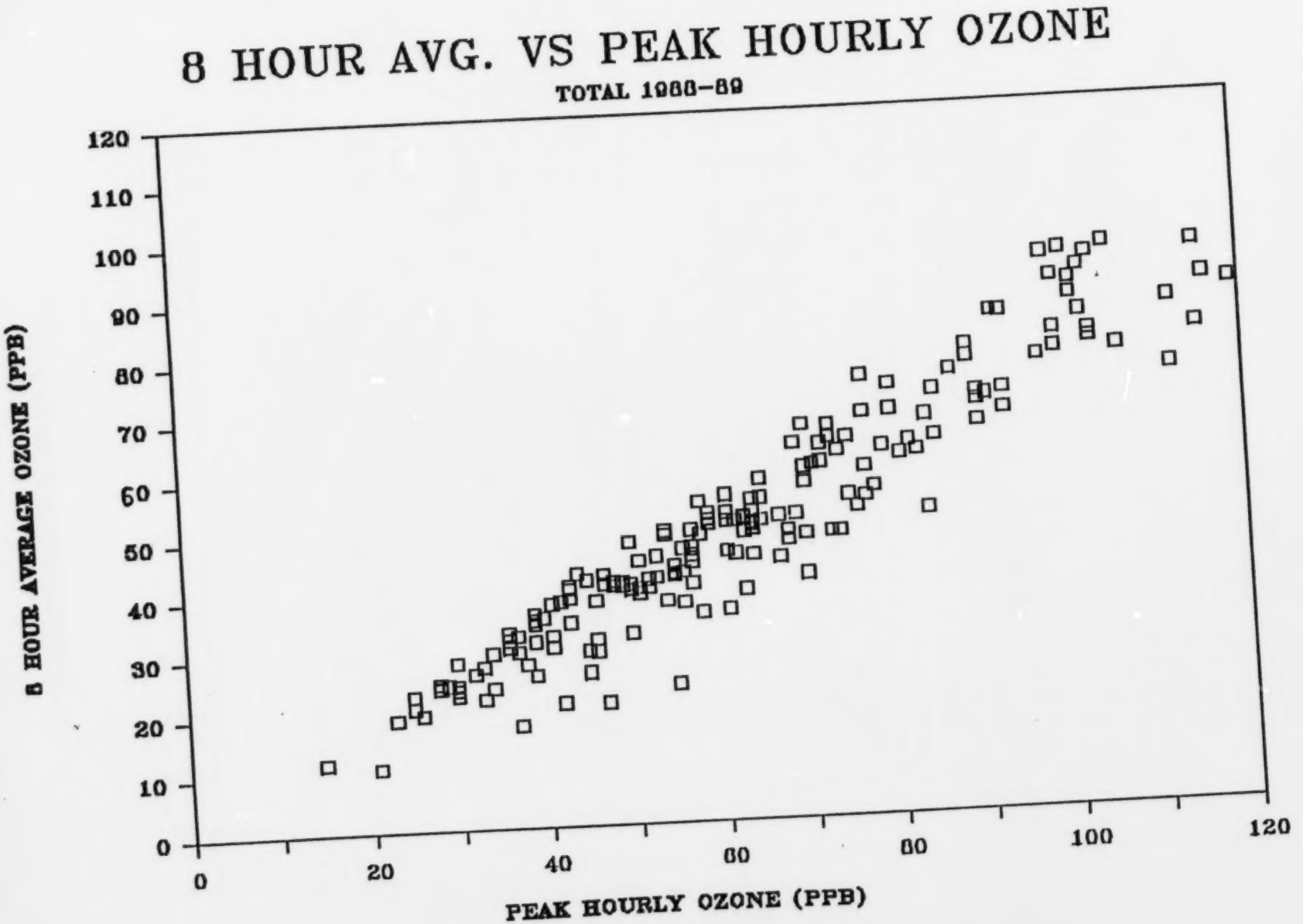

FIGURE 12: 8 Hour Average Versus Peak Hourly Ozone
Total, 1988-89

7. SUMMARY AND CONCLUSIONS

This study has determined that the levels of ozone in Metropolitan Toronto increases on LRT days. These increases in ozone averaged approximately 32% (26 ppb) and peaks as high as 49% (38 ppb) were noted. These results are compared with Wolff and Lioy (1978), who concluded by a similar means that the contribution of external sources to a Connecticut location during high ozone days, was as much as 75 ppb, and Prior et al. (1981) reported the LRT contribution to St. Louis was 36 ppb.

Multiple regression equations were determined relating the peak hour ozone levels with the same day maximum temperature, the average daytime windspeed, the cloud opacity at Pearson International Airport and the peak hour ozone concentration at the Simcoe rural station for the previous day, for LRT and non-LRT days in 1988 and 1989. Data for 1987 were used to validate the statistically determined relationships. These equations have proven to be reasonably good predictors of peak ozone levels in the Metropolitan Toronto area.

The study also indicated that Ontario's 80 ppb one-hour average regulatory limit cannot be used as a surrogate for an eight-hour average health standard. The World Health Organization Guidelines recommend 50 to 60 ppb for an eight-hour average level of ozone for the protection of human health.

Similar studies could be carried out in the future to determine regression equations for peak hourly ozone for other cities of Southern Ontario, for both LRT and non-LRT days. The regression equations can be used to predict the peak ozone levels and the associated AQI for each location. A good suggestion by a Ministry Scientist is to use the previous day's maximum ozone level at the C.N. Tower elevated station as a prediction variable. This could be tested in a future study.

8. REFERENCES

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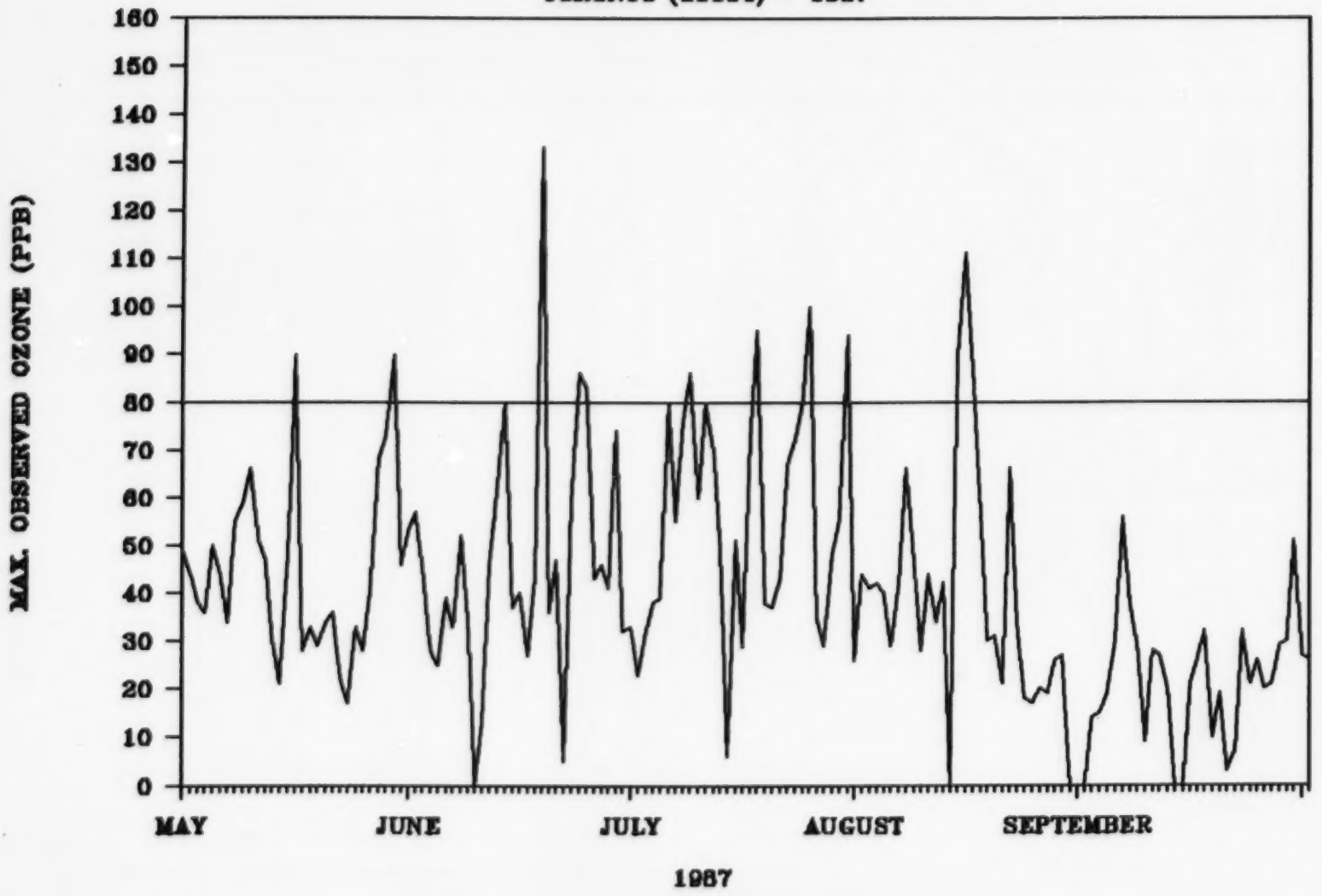
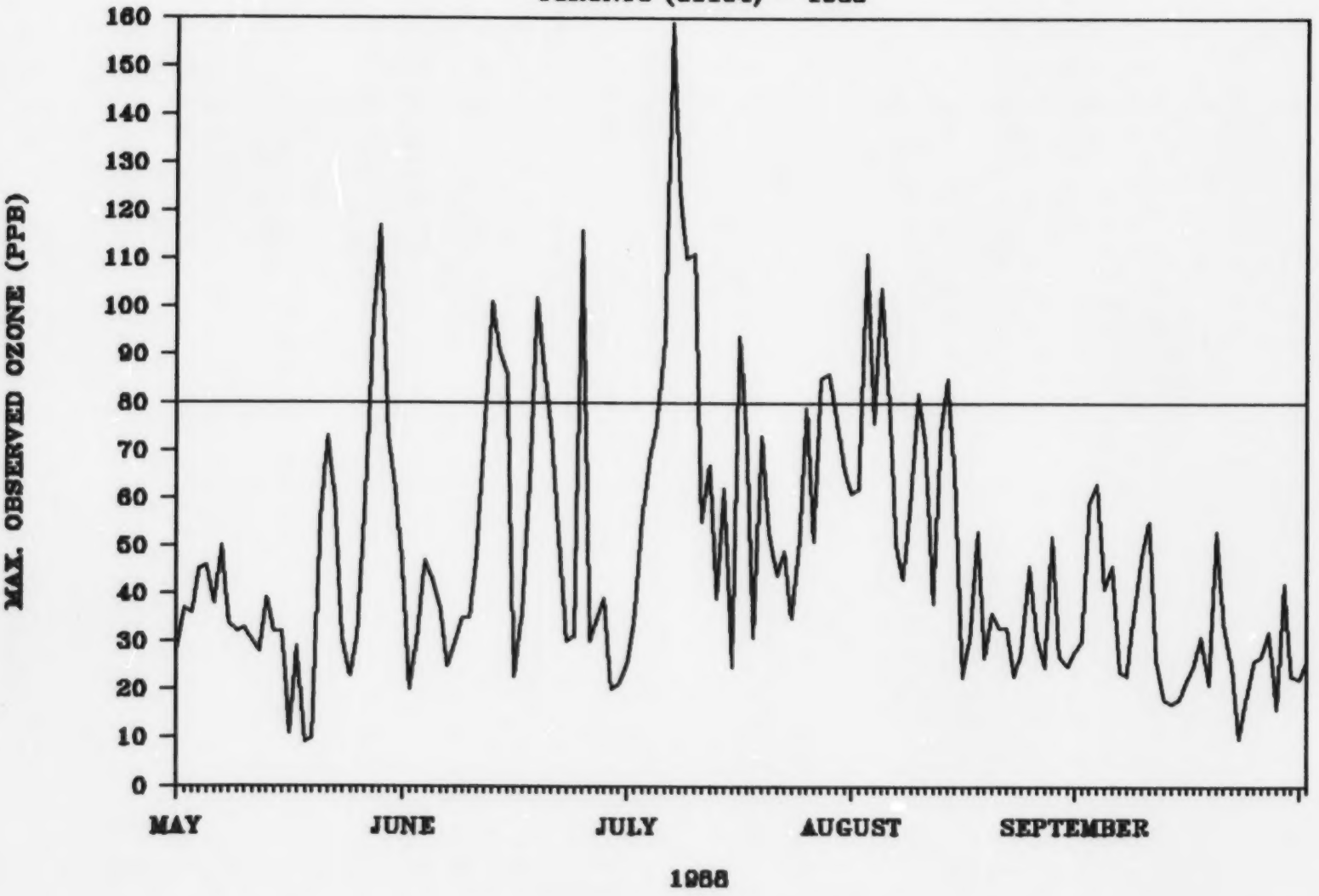
APPENDIX A

Maximum Observed Ozone

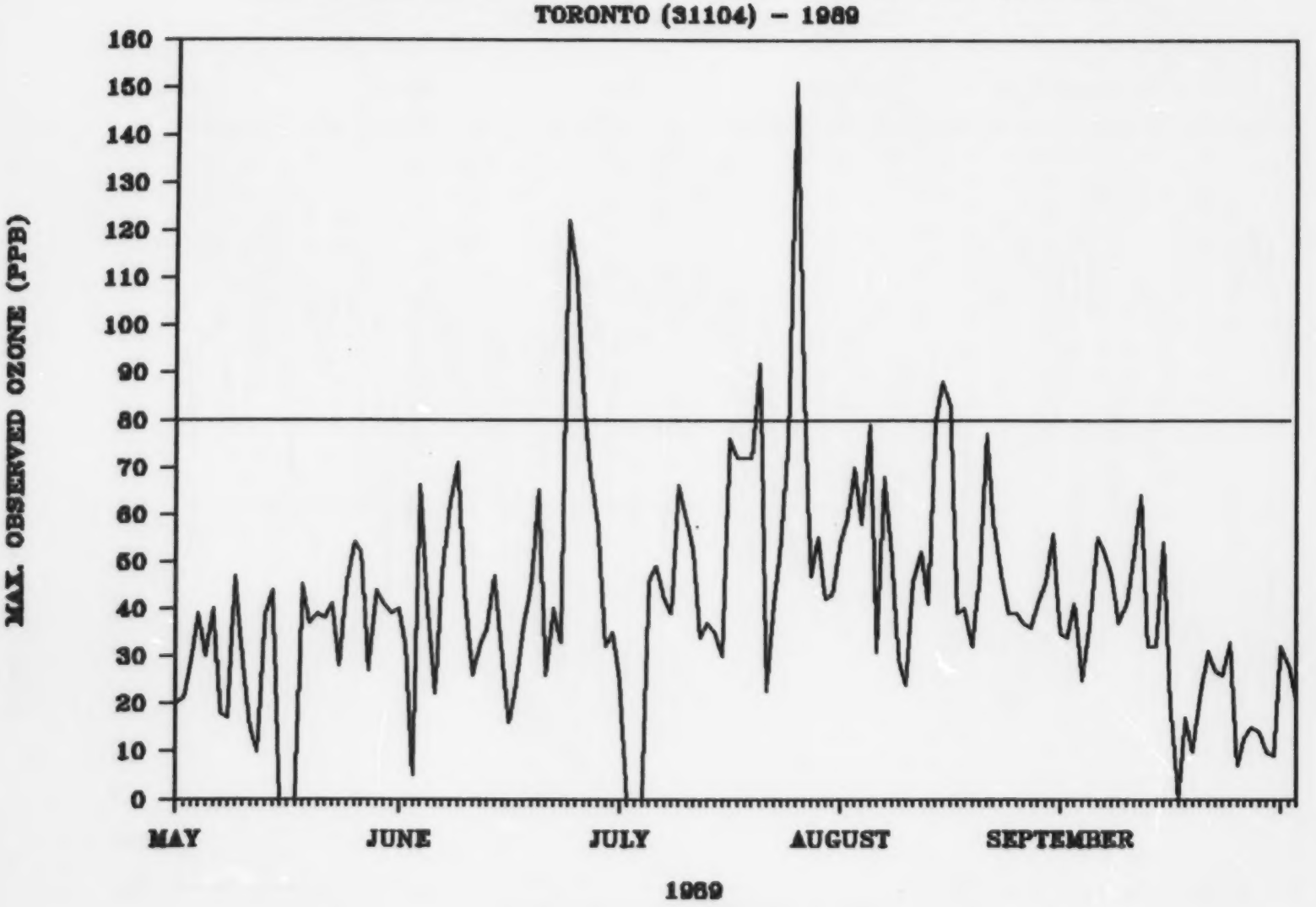
MAXIMUM OBSERVED OZONE (PPB)



MAXIMUM OBSERVED OZONE (PPB)

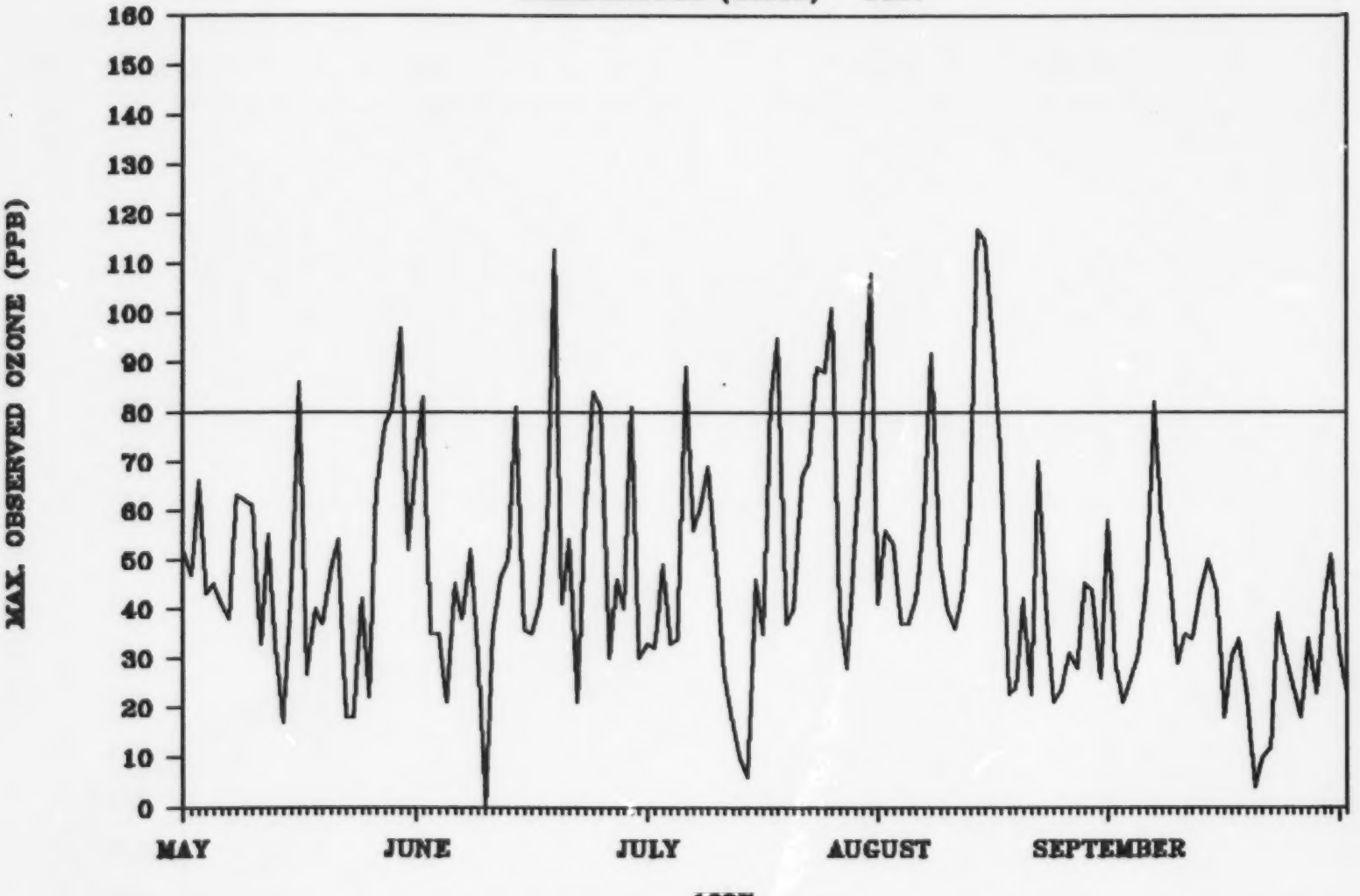


MAXIMUM OBSERVED OZONE (PPB)

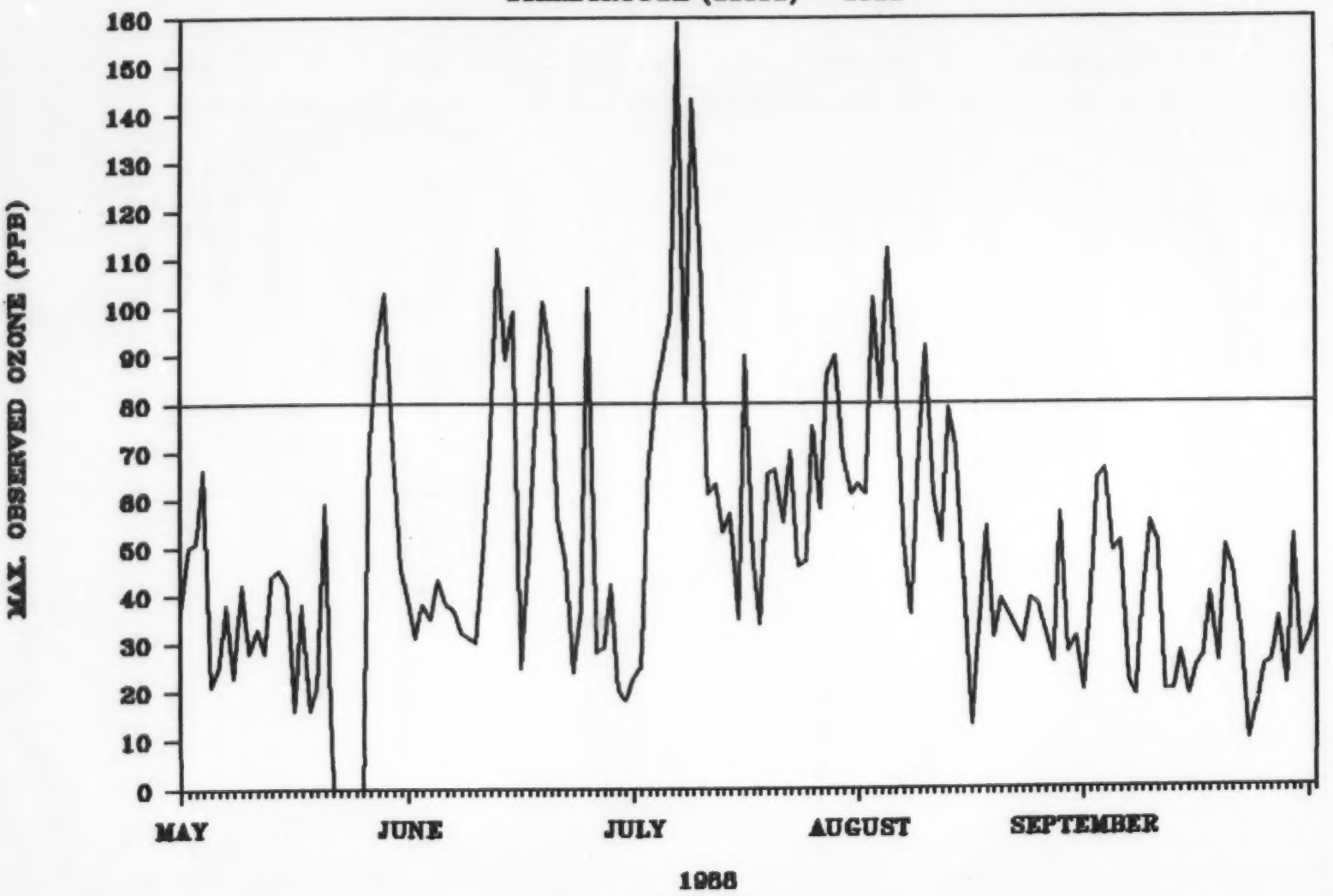


MAXIMUM OBSERVED OZONE (PPB)

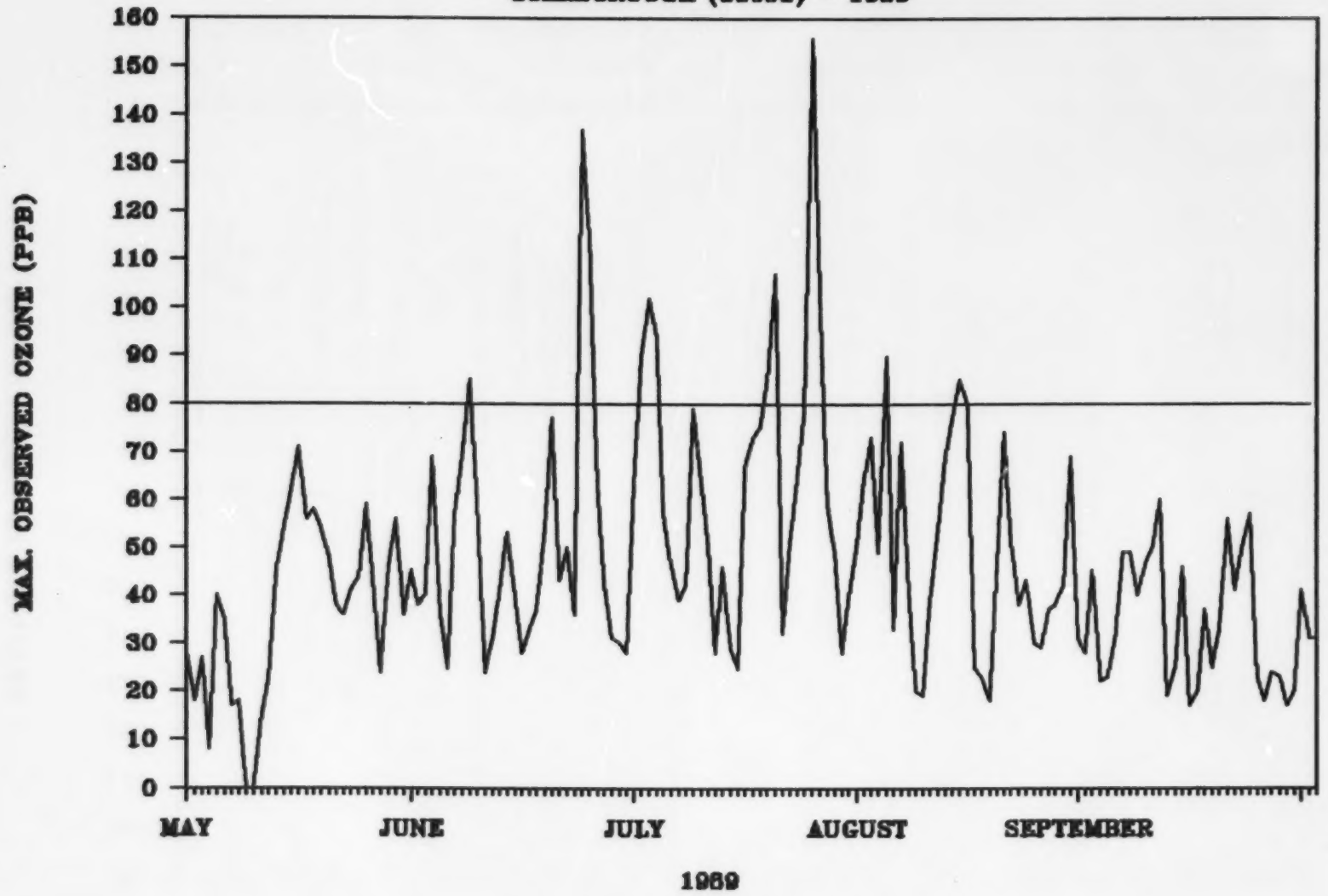
SCARBOROUGH (33003) – 1987

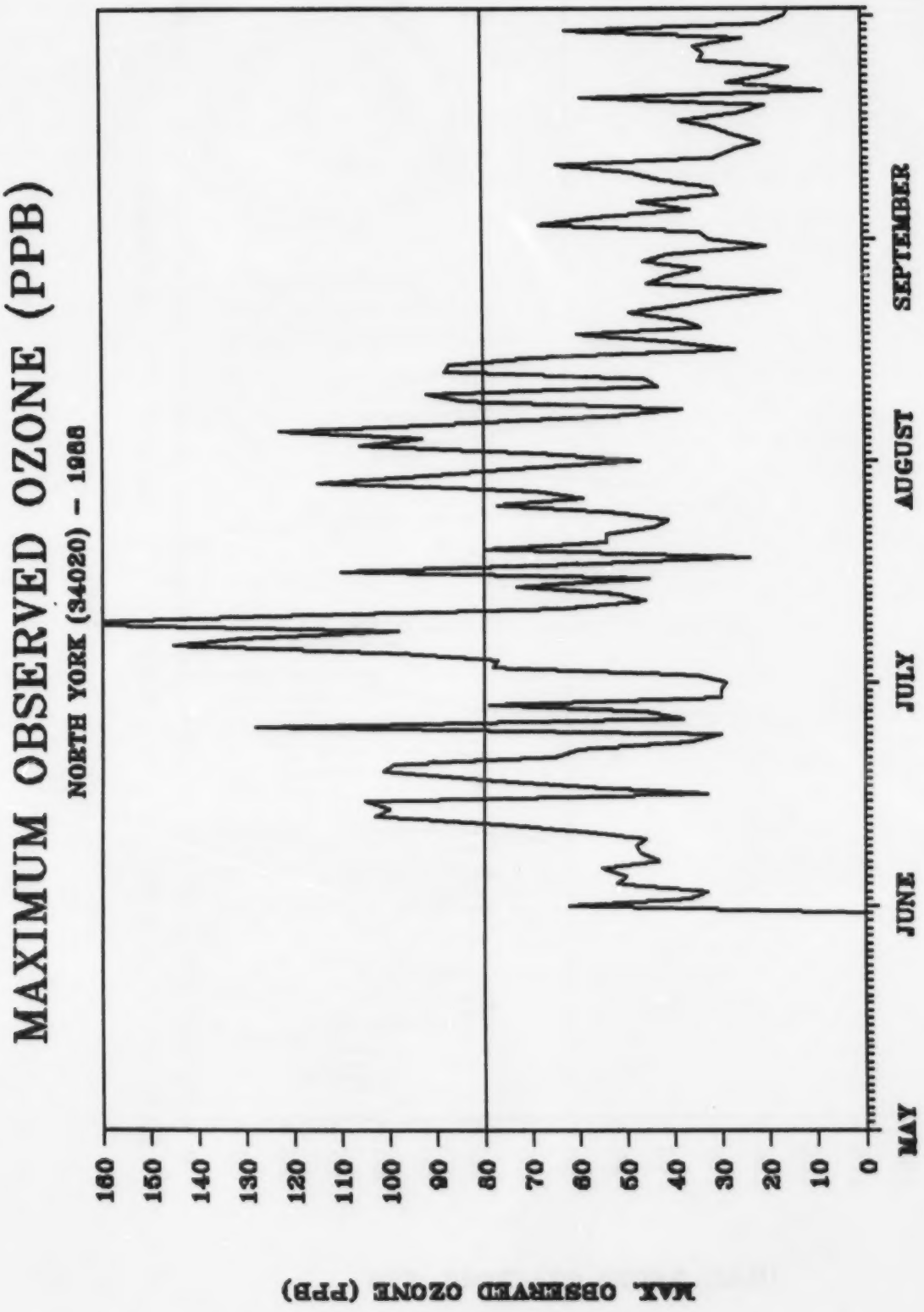


MAXIMUM OBSERVED OZONE (PPB)

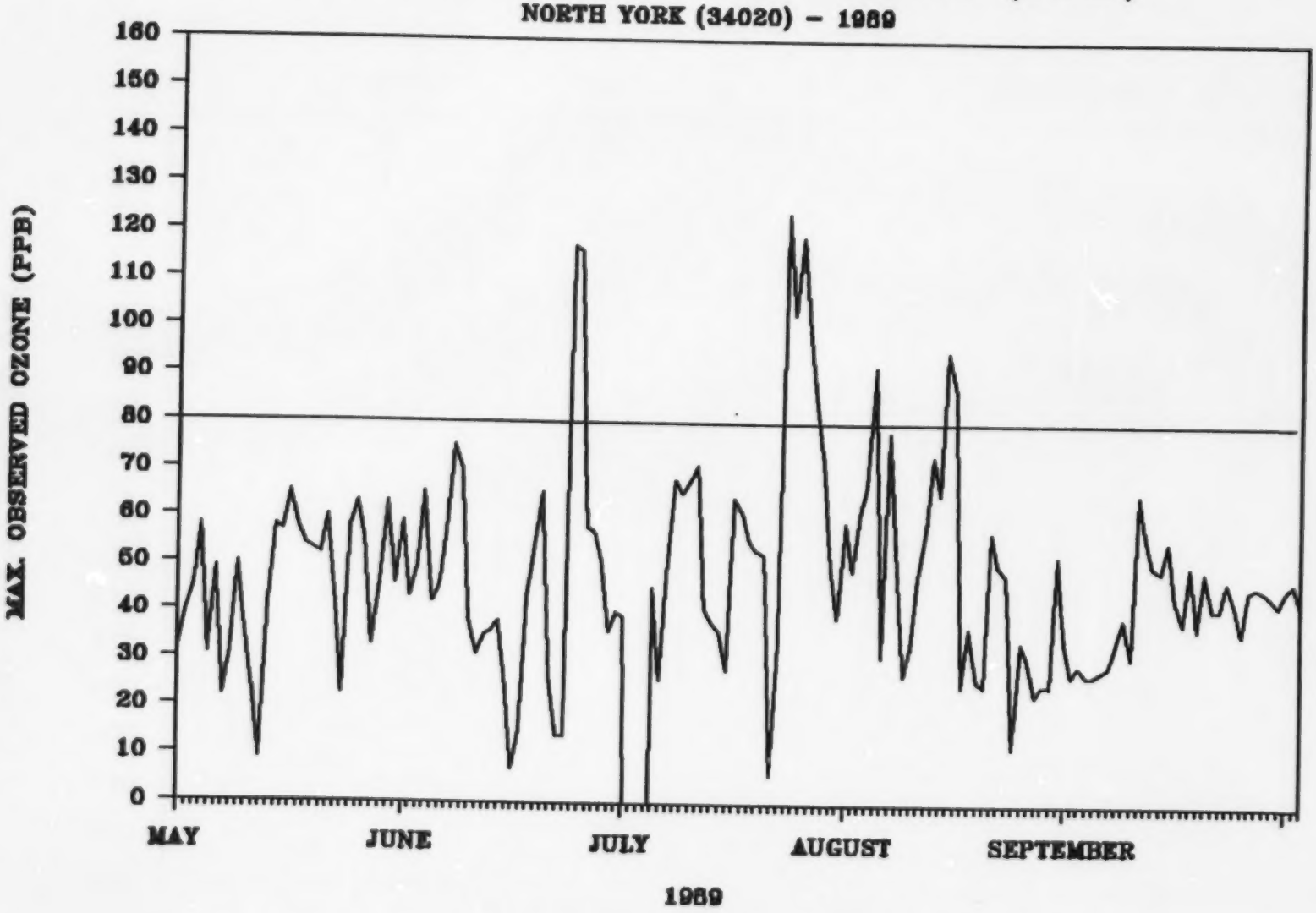


MAXIMUM OBSERVED OZONE (PPB)




MAXIMUM OBSERVED OZONE (PPB)
NORTH YORK (34020) - 1988
MAX. OBSERVED OZONE (PPB)
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
MAY
JUNE
JULY
AUGUST
SEPTEMBER
1988

MAXIMUM OBSERVED OZONE (PPB)



APPENDIX B

Number of Ozone Potential Days

NUMBER OF OZONE–POTENTIAL DAYS